Successive Continuation for Locating Connecting Orbits.

E. J. Doedel*, M. J. Friedman†and B. I. Kunin‡

*Computer Science Department, Concordia University, Montreal,
Quebec, H3G 1M8 Canada

†,‡Department of Mathematical Sciences, University of Alabama
in Huntsville, Huntsville, AL 35899

Abstract

A successive continuation method for locating connecting orbits in parametrized systems of autonomous ODEs is considered. A local convergence analysis is presented and several illustrative numerical examples are given.

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1   Introduction

The existence of a trajectory connecting equilibrium points of an ODE, a *homoclinic orbit* or *heteroclinic orbit*, also called *connecting orbit is* of significance in a variety of applications. Connecting orbits often arise as traveling wave solutions of parabolic and hyperbolic PDEs., e.g., in combustions models [2]. They have been shown to underlie intermittency phenomena in fluid

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mechanics [1], "bursting" in models of biological cells [30], chaotic vibration of structures [29], and chaotic behavior of electronic circuits, [9, 18, 19], light pulses in fiber optics [28], and chemical reactions [24]. The corresponding numerical problem is that of finding solutions $(u(t), \lambda)$ of the system of autonomous ODEs

$$u'(t) - f(u(t), \lambda) = 0, \quad u(\cdot), f(\cdot, \cdot) \in \mathbb{R}^n, \lambda \in \mathbb{R}^{n_\lambda}, \quad (1.1\text{a})$$
$$\lim_{t \to -\infty} u(t) = u_0, \quad \lim_{t \to +\infty} u(t) = u_1. \quad (1.1\text{b})$$

Most algorithms for computing connecting orbits reduce (1.1) to a boundary value problem on a finite interval using linear or higher order approximations of stable and unstable manifolds near u_0 and u_1, respectively. We studied and applied such a method in [13] and generalized it in [21]. An alternate convergence analysis of the method is given by Schecter [33]. The basic method of choosing appropriate boundary conditions dates back to Lentini and Keller [27]. A closely related procedure, which uses generalized eigenspaces for $f_u^T(u_0, \lambda)$ and $f_u^T(u_1, \lambda)$ to construct the relevant projections, was developed by Beyn [3, 4] and used by Champneys and Kuznetsov in their recent work on locating higher codimension homoclinic orbit bifurcations [7]. A shooting method for computing connecting orbits has been used by Rodríguez-Luis *et al* [31]. For parameter superconvergence results see the recent work of Sandstede [32].

We considered the case of center manifold in [20, 22]. Champneys, Kuznetsov, and Sandstede have also generalized the algorithm in [7] to the case of non-hyperbolic equilibria [8]. Both, hyperbolic and nonhyperbolic equilibria are considered by Canale [6], using multiple shooting for discretizing the approximate truncated problem, together with a new a new technique for evaluating partial derivatives in the boundary conditions.

In this paper we present a local convergence analysis of the *successive continuation method* for *locating* connecting orbits. This method aims at computing a connecting orbit when there is a region of uncertainty for the parameter values, which is the case in most practical problems. In contrast, most previous work is concerned with the *continuation* of connecting orbits, given a sufficiently accurate starting connecting orbit.

Assume that u_0 and u_1 are hyperbolic fixed points of the vector field f, and that the local unstable manifold $W_{loc}^u(u_0)$ at u_0 has dimension n_0, and that the local stable manifold $W_{loc}^s(u_1)$ at u_1 has dimension n_1. Let S_0 and S_1 denote the tangent planes to $W_{loc}^u(u_0)$ and $W_{loc}^s(u_1)$, respectively. In the

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finite interval approximation, the scaled independent variable takes values in $[0, 1]$. A general outline of the full algorithm for locating and continuing connecting orbits is then as follows:

(I) *Time integration to get an initial orbit.* Typically, this gives a very inaccurate "approximation" of a connecting orbit with either $(u(0)-u_0) \in S_0$ or $(u(1)-u_1) \in S_1$. This step can be done by continuation with the "period", i.e., the total integration time, as parameter.

(II) *Locate a connecting orbit.* Use a sequence of homotopies ("successive continuation") that lead to an orbit with both $(u(0) - u_0) \in S_0$ and $(u(1) - u_1) \in S_1$.

(III) *Increase the accuracy.* Use continuation to further increase the period of the approximate connecting orbit.

(IV) *Continue the connecting orbit.* If desired, compute an entire family of approximate connecting orbits.

In this paper we are primarily concerned with Step (II). In Section 2 we formulate the approximate problem and a successive continuation algorithm. This algorithm is implemented in a general code based on the continuation package AUTO [17] and is used to compute the examples in Section 4 below. In Section 3 we prove a local result, namely that the successive continuation algorithm has an open neighborhood of convergence. More precisely, we show that for any point in this neighborhood there exists a continuous piecewise smooth homotopy leading to the solution. Section 4 contains examples. In Section 5 we conclude with a discussion of the applicability and limitations of the algorithm.

In our original algorithm for continuing connecting orbits [13, 20] we included the eigenvectors as unknowns in the full system to be solved at each continuation step. This can lead to an ill-conditioned system in the case of a nearly defective eigenvalue, eigenvectors becoming nearly linearly dependent. In the present paper we use orthonormal bases to construct the appropriate projections associated with the real Schur factorization [23] of $f_u(u_0, \lambda)$ and $f_u(u_1, \lambda)$ or their transposes. This procedure is more accurate and stable.

We first realized the power of the successive continuation approach for locating connecting orbits when trying to find a homoclinic orbit in a singular perturbation problem [15]. For application to a singularly perturbed sine-Gordon model of the Josephson junctions and to the Hodgkin-Huxley equations see [14]. The basic idea was also used by Champneys and Kuznetsov to locate homoclinic orbit in Chua's electronic circuit and in the FitzHugh-Nagumo equations [7]. In the context of optimization, the approach is also

used in the tutorial papers [16].

2 Description of the algorithm

In addition to the requirement that the fixed points u_0 and u_1 be hyperbolic, we assume that the eigenvalues of $f_u(u_0, \lambda)$ and $f_u(u_1, \lambda)$, respectively, satisfy

$$\begin{align}
\operatorname{Re}\mu_{0,n} &\leq \ ... \leq \operatorname{Re}\mu_{0,n_0+1} < 0 < \mu_{0,1} < \operatorname{Re}\mu_{0,2} \leq ... \leq \operatorname{Re}\mu_{0,n_0}, &\text{(2.1a)} \\
\operatorname{Re}\mu_{1,1} &\leq \ ... \leq \operatorname{Re}\mu_{1,n_1} < 0 < \operatorname{Re}\mu_{1,n_1+1} \leq ... \leq \operatorname{Re}\mu_{1,n} &\text{(2.1b)}
\end{align}$$

The method can be extended to the case $\mu_{0,1} = 0$, as in [6, 8]. It also extends to the cases of complex and multiple $\mu_{0,1}$ by a modification of Step 0, Eq. (2.13) of the algorithm (see Section 4.3 for an example). The algorithm requires evaluation of various projections onto tangent subspaces at u_0 and u_1. We construct these projections using the real Schur factorizations [23]

$$f_u(u_0, \lambda) = Q_0 T_0 Q_0^T, \tag{2.2}$$

and

$$f_u(u_1, \lambda) = Q_1 T_1 Q_1^T, \tag{2.3}$$

of $f_u(u_0, \lambda)$ and $f_u(u_1, \lambda)$, respectively. The factorization (2.2) has been chosen so that, in the real case, the eigenvalues $\mu_{0,1}, ..., \mu_{0,n_0}$ appear in the upper left corner of T_0. In the complex case the corresponding 2×2 blocks for each complex congugate pair appear. A similar choice applies to the eigenvalues $\mu_{1,1}, ..., \mu_{1,n_1}$ and T_1 in the factorization (2.3). $Q_0 = [q_{0,1}...q_{0,n}]$ and $Q_1 = [q_{1,1}...q_{1,n}]$ are orthogonal, and T_0 and T_1 are upper quasi-triangular (1-by-1 and 2-by-2 blocks on their diagonals). Then the first n_0 columns $q_{0,1}, ..., q_{0,n}$ of Q_0 form an orthonormal basis of the right invariant subspace S_0 of $f_u(u_0, \lambda)$, corresponding to $\mu_{0,1}, ..., \mu_{0,n_0}$, and the last $n - n_0$ columns $q_{0,n_0+1}, ..., q_{0,n}$ of Q_0 form an orthonormal basis of the orthogonal complement $S_0^\perp$. Similarly, the first n_1 columns $q_{1,1}, ..., q_{1,n}$ of Q_1 form an orthonormal basis of the right invariant subspace S_1 of $f_u(u_1, \lambda)$, corresponding to $\mu_{1,1}, ..., \mu_{1,n_1}$, and the last $n - n_1$ columns $q_{1,n_1+1}, ..., q_{1,n}$ of Q_1 form an orthonormal basis of the orthogonal complement $S_1^\perp$.

Approximate problem.

The approximate finite interval problem is now as follows: given $\epsilon_0 = \epsilon_0^* \in \mathbb{R}_+$, "small", $T \in \mathbb{R}_+$, "large", find a solution

$$(u^*, \lambda^*, u_0^*, u_1^*, d_0^*, d_1^*, \epsilon_1^*, Q_0^*, Q_1^*, T_0^*, T_1^*),$$

where $u^* \in C^1([0,1]), \mathbb{R}^n), \lambda^* \in \mathbb{R}^{n_\lambda}, u_0^*, u_1^*, d_0^*, d_1^*, \in \mathbb{R}^n, \epsilon_1^*$ small, $Q_0^*, Q_1^*, T_0^*, T_1^* \in \mathbb{R}^n \times \mathbb{R}^n$, of the time-scaled differential equation

$$u'(t) - Tf(u(t), \lambda) = 0, \ 0 < t < 1, \tag{2.4}$$

subject to stationary state conditions

$$f(u_0, \lambda) \ = \ 0, \tag{2.5a}$$
$$f(u_1, \lambda) \ = \ 0, \tag{2.5b}$$

left boundary conditions

$$u(0) = u_0 + \epsilon_0 d_0, \tag{2.6a}$$
$$\mid d_0 \mid = 1, \tag{2.6b}$$
$$d_0 \cdot q_{0,n_0+j} = 0, \ j = 1, ..., n - n_0, \tag{2.6c}$$

right boundary conditions

$$u(1) = u_1 + \epsilon_1 d_1, \tag{2.7a}$$
$$\mid d_1 \mid = 1, \tag{2.7b}$$
$$\tau_j \quad \equiv \quad d_1 \cdot q_{1,n_1+j} = 0, \ j = 1, ..., n - n_1, \tag{2.8}$$

with real Schur factorization of $f_u(u_0, \lambda)$

$$f_u(u_0, \lambda) q_{0,i} = \sum_{j=1}^n q_{0,j} t_{j,i}^0, \ \ i = 1, ..., n, \tag{2.9a}$$

conditions for Q_0 to be orthogonal

$$q_{0,i}^T q_{0,j} = \delta_{i,j}, \quad i = 1, ..., j, \ j = 1, ..., n, \tag{2.9b}$$

real Schur factorization of $f_u(u_1, \lambda)$

$$f_u(u_1, \lambda) q_{1,i} = \sum_{j=1}^n q_{1,j} t_{j,i}^1, \ \ i = 1, ..., n, \tag{2.10a}$$

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and conditions for Q_1 to be orthogonal

$$q_{1,i}^T q_{1,j} = \delta_{i,j}, \quad i = 1, ..., j, \; j = 1, ..., n. \tag{2.10b}$$

Here the matrix $T_\delta = [t_{j,i}^\delta]$, $\delta = 0, 1$, is upper quasi-triangular with all elements below the subdiagonal equal to zero. During each continuation step its $n(n+1)/2$ elements above the subdiagonal vary, while the remaining $n-1$ elements on the subdiagonal are either fixed at zero or vary. In the latter case nearby diagonal elements are equated. Specifically, we have the following: each 1-by-1 block $t_{i,i}^\delta$ on the diagonal is a real eigenvalue, and each 2-by-2 block on the diagonal $\begin{bmatrix} t_{i,i}^\delta & t_{i,i+1}^\delta \\ t_{i+1,i}^\delta & t_{i+1,i+1}^\delta \end{bmatrix}$ corresponds to a complex conjugate pair, where $t_{i+1,i+1}^\delta = t_{i,i}^\delta$ is the real part of the eigenvalue and $t_{i,i+1}^\delta = -t_{i+1,i}^\delta$ is the imaginary part. In the process of continuation we have the following special cases: (i) if all eigenvalues are real and distinct then we let all entries on and above the main diagonal vary, while the entries on the subdiagonal are fixed at value zero; (ii) if we have a complex conjugate pair then we add the equation $t_{i+1,i+1}^\delta = t_{i,i}^\delta$ and let $t_{i+1,i}^\delta$ vary, (iii) if we have a double real eigenvalue then we can choose either of the preceding options. To summarize, we have

$$\begin{aligned} \text{if } t_{i+1,i+1}^0 \; &\neq \; t_{i,i}^0 \text{ set } t_{i+1,i}^0 = 0, \text{ else set } t_{i+1,i+1}^0 = t_{i,i}^0 \text{ and vary } t_{i+1,i}^0, \\ i \; &= \; 1, ..., n-1, \end{aligned} \tag{2.9c}$$

and similarly

$$\begin{aligned} \text{if } t_{i+1,i+1}^1 \; &\neq \; t_{i,i}^1 \text{ set } t_{i+1,i}^1 = 0, \text{ else set } t_{i+1,i+1}^1 = t_{i,i}^1 \text{ and vary } t_{i+1,i}^1, \\ i \; &= \; 1, ..., n-1. \end{aligned} \tag{2.10c}$$

We remark that a drawback in the earlier version of our algorithm was its inability to compute through double eigenvalues: we had to stop at double real eigenvalues and restart with a newly -defined continuation algorithm. The present method overcomes this problem: one just fixes appropriate parameters and frees other appropriate parameters (cf. steps 3 and 4 in Section 4.2).

The above constitutes n differential equations with $n_c = 3n^2 + 7n + 2 - n_0 - n_1$ constraints and $n_v = 3n^2 + 5n + n_\lambda + 1$ scalar variables. Generically, it is necessary that $n_c - n_v = n$, in order for the system (2.4) - (2.10) to have a unique solution. This gives the relation $n_\lambda = n - (n_0 + n_1) + 1$.

By a slight modification of the analysis in [21], using a version of the implicit function theorem used, e.g., in Beyn [3], it is easy to show, under appropriate transversality conditions, for T large enough and ϵ_0^* small enough, that the system (2.4) - (2.10) has a unique solution which is a good approximation to the solution of (1.1). Note that since in the present case we look for only one connecting orbit rather than a branch of connecting orbits, the dimension of the parameter vector λ is one less than in [21]. We also note that the proof in [21] is for the approximate problem in the same Banach space as the exact problem and that the result is independent of the particular implementation, and hence applies to the algorithmic implementation (2.1) - (2.6b) in [21] as well as to (2.4) - (2.10) in the present paper.

Algorithm for locating a connecting orbit.

The solution to the above system is found via a sequence of homotopies that locate successive zero intercepts of the τ_j, in

$$\tau_j - d_1 \cdot q_{1,n_1+j}(u_1, \lambda) = 0, \; j = 1, ..., n - n_1, \qquad (2.11)$$

(cf. equation (2.8)). In each homotopy step we compute a *branch*, i.e., a one-dimensional manifold, of solutions. For this we must have $n_c - n_v = n - 1$, and hence $n_\lambda = n - (n_0 + n_1) + 2; \; n_\lambda \geq 0$.

Let $S_{0,k}, \; k = 1, ..., n_0$, be the right invariant subspace of $f(u_0, \lambda_0)$ corresponding to the eigenvalues $\mu_{0,1}, ..., \mu_{0,k}$. Then the first k columns $q_{0,1}, ..., q_{0,k}$ of Q_0 form an orthonormal basis of $S_{0,k}$. Initially we replace (2.6) by the equivalent equations

$$u(0) = u_0 + \epsilon_0 \sum_{j=1}^{n_0} c_j q_{0j}, \qquad (2.12a)$$

$$\sum_{j=1}^{n_0} c_j^2 = 1. \qquad (2.12b)$$

Step 0. Initialize the problem parameter vector λ, and set the algorithm parameters ϵ_0 and T to small, positive values, so that $u(t)$ is approximately constant on $[0, T]$. Set $d_0 = q_{01}$,

$$u(t) = u_0 + \epsilon_0 \; d_0, \quad 0 \leq t \leq 1, \qquad (2.13)$$

$\epsilon_1 = |u(1) - u_1|, \; d_1 = (u(1) - u_1)/\epsilon_1, c_1 = 1$, and $c_2 = ... = c_{n_0} = 0$. Here the initial direction of the orbit is typically chosen along the eigenvector of the

weakest unstable eigenvalue, $d_0 = q_{01}$, which implies (2.6), i.e. $u(0) - u_0 \in S_0$.

Step 1.   Compute a solution branch to the system (2.4), (2.7), (2.11), (2.12a), in the direction of increasing T, until $u(1)$ reaches an ϵ_1-neighborhood of u_1, for some $\epsilon_1 > 0$. Scalar variables are $T, \epsilon_1 \in \mathbb{R}, d_1 \in \mathbb{R}^n, \tau \in \mathbb{R}^{n-n_1}$. There are n differential equations with $n_c = 3n - n_1 + 1$ constraints and $n_v = 2n - n_1 + 2$ scalar variables, and hence $n_c - n_v = n - 1$. This initial solution is normally a very inaccurate approximation of the solution of (2.4) - (2.10) since, in general, the τ_j in (2.11) will be nonzero and hence $u(1) - u_1 \notin S_1$. In practice one typically continues until ϵ_1 stops decreasing. Its value is then not necessarily small, but the successive continuation procedure is intended to work even then (see also Section 5).

Step 2 (for $\mathbf{n_0 > 1}$), $\mathbf{k = 2}$.   Keep T fixed and free c_1 and c_2, i.e., we let $u(0)$, which had been confined to $S_{0,1}$ in Step 1, now run through $S_{0,2}$. More precisely, we compute a branch of solutions to the system (2.4), (2.7), (2.11), (2.12) to locate a zero of, say, τ_1. Free scalar variables are $\epsilon_1, c_1, c_2 \in \mathbb{R}, d_1 \in \mathbb{R}^n, \tau \in \mathbb{R}^{n-n_1}$. There are n differential equations with $n_c = 3n - n_1 + 2$ constraints and $n_v = 2n - n_1 + 3$ scalar variables, and hence $n_c - n_v = n - 1$.

     (for $\mathbf{n_0 > 2}$), $\mathbf{k = 3, ..., n_0}$.   Keep T and $\tau_j = 0, j = 1, ...k - 2$, fixed. Also fix one more component of τ, say τ_{k-2}, which reached value zero in the previous step. Thus we now let $u(0) - u_0$, which had been confined to $S_{0,k-1}$, run through $S_{0,k}$. More precisely, we compute a branch of solutions to the system (2.4), (2.7), (2.11), (2.12) to locate zero of, say, τ_{k-1}. Free scalar variables are $\epsilon_1, c_1, ..., c_k, \tau_{k-1}, ..., \tau_{n-n_1} \in \mathbb{R}, d_1 \in \mathbb{R}^n$. There are n differential equations with $n_c = 3n - n_1 + 2$ constraints and $n_v = 2n - n_1 + 3$ scalar variables, and hence $n_c - n_v = n - 1$.

In the following steps, λ also varies. For the purpose of implementation, (2.12) is better than (2.6), but the latter is more stable when eigenvalues coalesce. There are examples where continuous dependence of q_{0j} on λ is lost, and where c_j oscillates. Consequently, starting with Step 3, we use (2.6) instead of (2.12), since (2.6) is more stable in this case.

Step 3, $\mathbf{k = n_0 + 1, ..., n_0 + n_\lambda \equiv n - n_1 + 1}$. The free parameters $c_1, ..., c_k \in \mathbb{R}$ are replaced by $d_0 \in \mathbb{R}^n$. Fix another component of τ, say, τ_{k-2}, which reached zero in the previous step, and free one more component of λ, say, λ_{k-n_0}. More precisely, we compute a branch of solutions to the system (2.4) - (2.7), (2.9) - (2.11). There are n differential equations with $n_c = 3n^2 + 7n + 2 - n_0 - n_1$ constraints and $n_v = 3n^2 + 6n + 3 - n_0 - n_1$ scalar variables, and hence $n_c - n_v = n - 1$.

In some of the examples below we use slight variations on the basic algo-

rithm in order to minimize the number of steps, which attests to its flexibility.

The above algorithm corresponds to Step (II) in the outline of the full algorithm for locating and continuing connecting orbits in Section 1. Step (IV) of that outline can now be described as follows.

Algorithm for continuing a connecting orbit.

Compute a branch of solutions to the system (2.4) - (2.10), where T, and all components of λ vary. Here $u(0) \in S_0$, $u(1) \in S_1$, T, and all components of λ vary. A phase condition

$$\int_0^1 (u'(t) - q'(t)) \cdot u''(t) \ dt = 0 \tag{2.14}$$

may be added if T is kept fixed and ϵ_0 and ϵ_1 are allowed to vary. Here $q(t)$ is a previously computed orbit on the branch.

Remark 1 *The factorizations (2.2), (2.3) can be computed at each continuation step using, for example, LAPACK, or by continuation. Continuation appears to be more robust. This is to be expected when the eigenvectors, and hence the Schur matrix, vary rapidly with a slow change of a continuation parameter, since in this case the pseudo-arclength step will automatically decrease to capture the transition. We also compared computing a connecting orbit via continuation and via factorizations in cases where the Schur matrices depend "smoothly" on the problem parameters. Computations using continuation were 10-20 times faster (due to larger continuation steps).*

Remark 2 *For the convenience of the reader, we summarize here some of the issues related to the algorithms for locating and continuing a connecting orbit, in this paper and in our earlier work. (1) The **Approximate problem** in here is to locate a connecting orbit, while the approximate problem in [21] is to continue a branch of connecting orbits. Hence the difference between two formulations. (2) Once a connecting orbit has been located, there are two basic methods to continue a branch of connecting orbits (see **Algorithm for continuing a connecting orbit** on p. 7): (a) T, and λ vary, while ϵ_0 and ϵ_1 are kept fixed; (b) T is kept fixed, ϵ_0 and ϵ_1 are allowed to vary, and a phase condition is added. Both types of continuation have their advantages and disadvantages. The advantage of (a) is that the accuracy of the computed orbits on the branch is the same (since ϵ_0 and ϵ_1 are fixed), while the advantage of (b) is that it often works (and works well) for more*

difficult cases (i.e. when the orbit changes rapidly during the continuation), when (a) fails or becomes extremely slow. See also the Remark in [13] which explains (b) in more detail.

Remark 3 *An alternate formulation.* *An alternate formulation using transposed matrices, as in [3, 4, 7, 27], results in a similar algorithm. The real Schur factorizations (2.2) and (2.3) are replaced by*

$$f_u^T(u_0, \lambda) = Q_0 T_0 Q_0^T \qquad (2.15)$$

and

$$f_u^T(u_1, \lambda) = Q_1 T_1 Q_1^T, \qquad (2.16)$$

respectively. Correspondingly, the system (2.4) - (2.10) is replaced by the system (2.4) - (2.6a,b), (2.7), and

$$d_0 \cdot q_{0,j} = 0, \ j = 1, ..., n - n_0, \qquad (2.17)$$

$$\tau_j \equiv d_1 \cdot q_{1,j} = 0, \ j = 1, ..., n - n_1, \qquad (2.18)$$

$$f_u^T(u_0, \lambda) q_{0,i} \ = \ \sum_{j=1}^{n} q_{0,j} t_{j,i}^0, \ \ i = 1, ..., n, \qquad (2.19a)$$

$$\text{if } t_{i+1,i+1}^0 \ \neq \ t_{i,i}^0 \text{ then set } t_{i+1,i}^0 = 0, \text{ else set } t_{i+1,i+1}^0 = t_{i,i}^0, \text{and } vary \ t_{i+1,i}^0,$$
$$i \ = \ 1, ..., n - 1, \qquad (2.19b)$$
$$q_{0,i}^T q_{0,j} \ = \ \delta_{i,j}, \ \ \ i = 1, ..., j, \ j = 1, ..., n, \qquad (2.19c)$$

$$f_u^T(u_1, \lambda) q_{1,i} \ = \ \sum_{j=1}^{n-n_1} q_{1,j} t_{j,i}^1, \ \ i = 1, ..., n, \qquad (2.20a)$$

$$\text{if } t_{i+1,i+1}^1 \ \neq \ t_{i,i}^1 \text{ then set } t_{i+1,i}^1 = 0, \text{ else set } t_{i+1,i+1}^1 = t_{i,i}^1, \text{and } vary \ t_{i+1,i}^1,$$
$$i \ = \ 1, ..., n - 1, \qquad (2.20b)$$
$$q_{1,i}^T q_{1,j} \ = \ \delta_{i,j}, \ \ \ i = 1, ..., j, \ j = 1, ..., n. \qquad (2.20c)$$

3 Convergence of the algorithm

The following notation will be used throughout this section:

$$n_\lambda = n + 1 - n_0 - n_1, \tag{3.1a}$$
$$n_\tau = n - n_1 = n_\lambda + n_0 - 1. \tag{3.1b}$$

In the system (2.4)-(2.10), equations (2.9)-(2.10) can be used to find numerically Q_0 and Q_1 as functions of u_0, λ and u_1, λ, respectively. This allows to treat (2.4)-(2.8) as a self-contained problem. Replace the problem (2.4)–(2.8) by an equivalent one

$$u'(t) - Tf(u(t), \lambda) = 0, \;\; 0 < t < 1, \tag{3.2}$$

$$f(u_0, \lambda) = 0, \tag{3.3a}$$
$$f(u_1, \lambda) = 0, \tag{3.3b}$$

$$|u(0) - u_0| = \epsilon_0, \tag{3.4}$$

$$\sigma_i \equiv (u(0) - u_0) \cdot q_{0, n_0 + i}(u_0, \lambda) = 0, \;\; i = 1, ..., n - n_0, \tag{3.5a}$$
$$\sigma_{n-n_0+i} \equiv (u(0) - u_0) \cdot q_{0, i+1}(u_0, \lambda) - \nu_i = 0, \;\; i = 1, ..., n_0 - 1, \tag{3.5b}$$

$$\tau_i \equiv (u(1) - u_1) \cdot q_{1, n_1 + i}(u_1, \lambda) = 0, \;\; i = 1, ..., n_\tau. \tag{3.6}$$

The equivalence is apparent, since the system (3.2)–(3.4), (3.5a), (3.6) becomes formally equivalent to the system (2.4)–(2.8) if appended by the equations

$$d_0 = (u(0) - u_0)/\epsilon_0, \tag{3.7a}$$
$$\epsilon_1 = |u(1) - u_1|, \tag{3.7b}$$
$$d_1 = (u(1) - u_1)/\epsilon_1, \tag{3.7c}$$

whereas (3.5b) merely defines the parameters ν_i. Notice that $\nu_i = c_{i+1}$, $i = 1, ..., n_0 - 1$, where c_i's appear in (2.12).

Definition *A set $\mathcal{A}$ in a Banach space X will be called an arc if there exists a Banach space Y and an open sets $U \subset X$, $V \subset Y$ and a C^1-diffeomorphism $F : U \to V$ such that $\mathcal{A} \subset U$ and $F(\mathcal{A})$ is a closed bounded rectilinear segment (a degenerate segment consisting of a single point is allowed).*

Remark 4 *Any arc $\mathcal{A}$ has finite length. Indeed, if $\gamma : [0,1] \to Y$ is a linear parametrization of the rectilinear segment $F(\mathcal{A})$, then $F^{-1} \circ \gamma$ is a smooth parametrization of $\mathcal{A}$ with continuous, hence bounded, velocity $v(s) = [F^{-1}]'(\gamma(s)) \circ \gamma'(s)$. Thus $(length\ of\ A) \leq \sup |v(s)|.$*

Introduce two Banach spaces, $X = C^1[0,1] \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^{n_\tau} = \{x = (U, \Lambda) : U = (u, u_0, u_1) \in C^1[0,1] \times \mathbb{R}^n \times \mathbb{R}^n, \; u \in C^1[0,1], u_0, u_1 \in \mathbb{R}^n, \; \Lambda = (\nu, \lambda) \in \mathbb{R}^{n_\tau}, \; \nu \in \mathbb{R}^{n_0-1}, \; \lambda \in \mathbb{R}^{n_\lambda}\}$ and $Y = C[0,1] \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R} \times \mathbb{R}^{n-1}$. Define $F : X \to Y$ by

$$F(U, \Lambda) = \left(u' - T f(u, \lambda), \; f(u_0, \lambda), \; f(u_1, \lambda), \; |u(0) - u_0|^2 - \epsilon_0^2, \; \sigma(U, \Lambda)\right), \tag{3.8}$$

where $\sigma : X \to \mathbb{R}^{n-1}$, $\sigma = (\sigma_1, ..., \sigma_{n-1})$ is defined by

$$\sigma_i(U, \Lambda) \;=\; (u(0) - u_0) \cdot q_{0, n_0+i}(u_0, \lambda), \quad i = 1, ..., n - n_0 \tag{3.9a}$$

$$\sigma_i(U, \Lambda) \;=\; (u(0) - u_0) \cdot q_{0, i+1-(n-n_0)}(u_0, \lambda) - \nu_{i-(n-n_0)}, \quad i = n - n_0 + 1, ..., n - 1. \tag{3.9b}$$

Also define $\tau : X \to \mathbb{R}^{n_\tau}$, $\tau = (\tau_1, ..., \tau_{n_\tau})$ by

$$\tau_j(U, \Lambda) = (u(1) - u_1) \cdot q_{1, n_1+j}(u_1, \lambda), \quad j = 1, ..., n_\tau. \tag{3.10}$$

Theorem *Define $F^{(j)} : X \to Y \times \mathbb{R}^{n_\tau}$, $F^{(j)} = \left(F_Y^{(j)}, F_1^{(j)}, ..., F_{n_\tau}^{(j)}\right)$, $j = 1, ..., n_\tau$, by*

$$F^{(j)}(U, \Lambda) \;=\; (F(U, \Lambda), \tau_1(U, \Lambda), ..., \tau_j(U, \Lambda), \Lambda_{j+1}, ..., \Lambda_{n_\tau}), \quad j = 1, ..., n_\tau - 1, \tag{3.11a}$$

$$F^{(n_\tau)}(U, \Lambda) \;=\; (F(U, \Lambda), \tau(U, \Lambda)). \tag{3.11b}$$

Assume that there exist $(U^*, \Lambda^*) \in X$ such that

$$F^{(n_\tau)}(U^*, \Lambda^*) = 0. \tag{3.12}$$

Assume also that for $j = 1, ..., n_\tau$, $F^{(j)}$ is a C^1-mapping in an open neighborhood of (U^*, Λ^*), and its Frechét derivative at (U^*, Λ^*) is an invertible bounded linear operator.

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Then there exists an open neighborhood V of (U^*, Λ^*) such that for any $(U^0, \Lambda^0) \in V \cap \{(U, \Lambda) : F(U, \Lambda) = 0\}$ *there exists a continuous piecewise smooth curve* $x(s) = (U(s), \Lambda(s))$, $s \in [0, 1]$, $x(0) = (U^0, \Lambda^0)$, $x(1) = (U^*, \Lambda^*)$ *with the following properties:*

(i) $x([0, 1]) \subset V$ *and consists of* n_τ *arcs, specifically, there exist numbers* $0 \le s_0 \le s_1 \le .. \le s_{n_\tau} = 1$ *such that each* $\mathcal{A}_k = x([s_{k-1}, s_k])$, $k = 1, ..., n_\tau$ *is an arc;*

(ii) for any $s \in [0, 1]$, $F(x(s)) = 0$ *;*

(iii) for any $k \in \{2, ..., n_\tau\}$, *if* $x \in \mathcal{A}_k$, *then* $\tau_1(x) = ... = \tau_{k-1}(x) = 0$;

(iv) for any $s \in [0, 1]$, *if* $\tau_k(x(s)) \ne 0$ *for some* $k \in \{1, ..., n_\tau - 1\}$, *then* $\Lambda_{k+1}(s) = \Lambda_{k+1}^0, ..., \Lambda_{n_\tau}(s) = \Lambda_{n_\tau}^0$.

The hypotheses of the Theorem which require that *Frechét derivatives of* $F^{(j)}$ *at the solution* (U^*, Λ^*) *are invertible bounded linear operators,* express the following transversality requirements. The surface $\{F = 0\}$ and the hypersurfaces $\{\tau_1 = 0\}, ..., \{\tau_{n_\tau} = 0\}$ intersect transversely at the solution (U^*, Λ^*); the same holds for the surface $\{F = 0\}$ and the hypersurfaces $\{\tau_1 = 0\}, ..., \{\tau_j = 0\}, \{\Lambda_{j+1} = \Lambda_{j+1}^*\}, ..., \{\Lambda_{n_\tau} = \Lambda_{n_\tau}^*\}$, for each $j = 1, ..., n_\tau - 1$. In particular, these requirements imply that, at the end of each step j $(j = 1, ..., n_\tau)$, τ_j crosses zero transversely.

Define

$$\Sigma_0 = \{x \in X : F(x) = 0\}, \quad \Sigma_i = \Sigma_0 \cap \bigcap_{k=1}^{i} \{x \in X : \tau_k(x) = 0\}, \quad i = 1, ..., n_\tau.$$
(3.13)

The following Lemma 1 may be interpreted as Lemma 2_j below for $j = n_\tau$. To emphasize this, the condition (iv) is included in Lemma 1 even though it is a trivial consequence of (iii). Incorporation of the case $j = n_\tau$ into the statement of Lemma 2_j would lead to a cumbersome formulation.

Lemma 1 *Let* F, τ, U^*, Λ^*, $F^{(n_\tau)}$ *satisfy the hypothesis of the Theorem. Then there exists an open neighborhood* W *of* (U^*, Λ^*) *such that for any* $(U^{n_\tau-1}, \Lambda^{n_\tau-1}) \in W \cap \Sigma_{n_\tau-1}$ *there exists a smooth curve* $x(s) = (U(s), \Lambda(s))$, $s \in [0, 1]$, $x(0) = (U^{n_\tau-1}, \Lambda^{n_\tau-1})$, $x(1) = (U^*, \Lambda^*)$ *with the following properties:*

(i) $x([0, 1]) \subset W$ *and is an arc;*

(ii) for any $s \in [0, 1]$, $F(x(s)) = 0$;

(iii) for any $k \in \{1, ..., n_\tau - 1\}$, $\tau_k(x(s)) = 0$ *for all* $s \in [0, 1]$.

(iv) for any $s \in [0, 1]$, *if* $\tau_k(x(s)) \ne 0$ *for some* $k \in \{1, ..., n_\tau - 1\}$, *then* $\Lambda_{k+1}(s) = \Lambda_{k+1}^{n_\tau-1}, ..., \Lambda_{n_\tau}(s) = \Lambda_{n_\tau}^{n_\tau-1}$;

Lemma 2$_j$ *Let $j \in \{1, ..., n_\tau - 1\}$ and let F, τ, U^*, Λ^*, $F^{(j)}$ satisfy the hypothesis of the Theorem. Assume that there exists an open neighborhood $W^{(j)}$ of (U^*, Λ^*) such that for any $(U^j, \Lambda^j) \in W^{(j)} \cap \Sigma_j$ there exists a continuous piecewise smooth curve $x^{(j)}(s) = (U^{(j)}(s), \Lambda^{(j)}(s))$, $s \in [0, 1]$, $x^{(j)}(0) = (U^j, \Lambda^j)$, $x^{(j)}(1) = (U^*, \Lambda^*)$ with the following properties:*

(i_j) $x^{(j)}([0, 1]) \subset W^{(j)}$ and consists of $n_\tau - j$ arcs, specifically, there exist numbers $0 \leq s_j^{(j)} \leq s_{j+1}^{(j)} \leq ... \leq s_{n_\tau}^{(j)} = 1$ such that each $\mathcal{A}_k^{(j)} = x^{(j)}([s_{k-1}^{(j)}, s_k^{(j)}])$, $k = j+1, ..., n_\tau$ is an arc;

(ii_j) for any $s \in [0, 1]$, $F\left(x^{(j)}(s)\right) = 0$;

(iii_j) for any $k \in \{j+1, ..., n_\tau\}$, if $x \in \mathcal{A}_k^{(j)}$, then $\tau_1(x) = ... = \tau_{k-1}(x) = 0$.

(iv_j) for any $s \in [0, 1]$, if $\tau_k\left(x^{(j)}(s)\right) \neq 0$ for some $k \in \{1, ..., n_\tau - 1\}$, then $\Lambda_{k+1}(s) = \Lambda_{k+1}^j, ..., \Lambda_{n_\tau}(s) = \Lambda_{n_\tau}^j$.

Then there exists an open neighborhood $W^{(j-1)}$ of (U^*, Λ^*) such that for any $(U^{j-1}, \Lambda^{j-1}) \in W^{(j-1)} \cap \Sigma_{j-1}$ there exists a continuous piecewise smooth curve $x^{(j-1)}(s)$, $s \in [0, 1]$, $x^{(j-1)}(0) = (U^{j-1}, \Lambda^{j-1})$, $x^{(j-1)}(1) = (U^*, \Lambda^*)$ which satisfies the conditions $(i) - (iv)$ above with j substituted by $j - 1$.

Proof of Theorem. Lemma 1 guarantees the existence of a neighborhood described in the hypothesis of Lemma 2$_{n_\tau-1}$ (take $W^{(n_\tau-1)} = W$). The conclusion of the latter assures the existence of a neighborhood described in the assumption of Lemma 2$_{n_\tau-2}$, and so on. At the end one finds that there exists a neighborhood $W^{(0)}$ described in the conclusion of Lemma 2$_1$. The properties of $W^{(0)}$ coincide with the requirements for V. Thus take $V = W^{(0)}$.

Proof of Lemma 1. By the Inverse Mapping Theorem [10, 26], applied to $F^{(n_\tau)}$ there exist open neighborhoods A, A' of (U^*, Λ^*) and $F^{(n_\tau)}(U^*, \Lambda^*) = 0$, respectively, such that the restriction $F^{(n_\tau)} : A \rightarrow A'$ has a continuously differentiable inverse $H : A' \rightarrow A$. Let B be an open ball in $Y \times \mathbb{R}^{n_\tau}$ centered at 0 and contained in A'. Define $W = H(B)$. Let $(U^{n_\tau-1}, \Lambda^{n_\tau-1}) \in W \cap \Sigma_{n_\tau-1}$. Define

$$x(s) = H(y(s)), \ s \in [0, 1], \tag{3.14}$$

where

$$y(s) = (y_Y(s), y_1(s), ..., y_{n_\tau}(s)) = (0_Y, 0, ..., 0, (1-s)\tau_{n_\tau}(U^{n_\tau-1}, \Lambda^{n_\tau-1})), \tag{3.15}$$

and 0_Y is the zero element in Y.

To see that x satisfies condition (i), notice that $y(s)$, $s \in [0,1]$, is a rectilinear segment connecting $y(0) = F^{(n_\tau)}(U^{n_\tau - 1}, \Lambda^{n_\tau - 1})$ to $y(1) = 0$. The latter is the center of the ball B and $F^{(n_\tau)}(U^{n_\tau - 1}, \Lambda^{n_\tau - 1}) \in B$. Therefore $y[0,1] \subset B$ (so, in particular, $H(y(s))$, $s \in [0,1]$, is well defined). We conclude that $x([0,1]) = H(y([0,1]))$ is an arc.

That $x(s)$ satisfies condition (ii) is clear from $F(x(s)) = F_Y^{(n_\tau)}(x(s)) = y_Y(s) = 0$, $s \in [0,1]$.

Notice that, for $k = 1, ..., n_\tau - 1$, $\tau_k(x(s)) = F_k^{(n_\tau)}(x(s)) = y_k(s) = 0$ for all $s \in [0,1]$, i.e. condition (iii) holds.

Condition (iv) is a trivial consequence of (iii).

Proof of Lemma 2$_j$. By the Inverse Mapping Theorem applied to $F^{(j)}$ there exist open neighborhoods A, A', of (U^*, Λ^*) and of $y^* = F^{(j)}(U^*, \Lambda^*) = \left(0_Y, 0, ..., 0, \Lambda_{j+1}^*, ..., \Lambda_{n_\tau}^* \right)$, respectively, such that $F^{(j)} : A \to A'$ has a continuously differentiable inverse $H : A' \to A$. Then $F^{(j)} \left(W^{(j)} \cap A \right) = H^{-1} \left(W^{(j)} \cap A \right)$ is open and contains y^* (since both $W^{(j)}$ and A are open, both contain (U^*, Λ^*), and H is continuous). Therefore there exists an open ball B in $Y \times \mathbb{R}^{n_\tau}$ centered at y^* and contained in $F^{(j)} \left(W^{(j)} \cap A \right)$. Set $W^{(j-1)} = H(B)$.

Let us verify that $W^{(j-1)}$ possesses the desired properties. Let $(U^{j-1}, \Lambda^{j-1}) \in W^{(j-1)} \cap \Sigma_{j-1}$. Define a parametrized curve $x(s)$ by

$$x(s) = H(y(s)), \ s \in [0,1], \tag{3.16}$$

where

$$y(s) = (y_Y(s), y_1(s), ..., y_{n_\tau}(s)) = \left(0_Y, 0, ..., 0, (1-s)\tau_j(U^{j-1}, \Lambda^{j-1}), \Lambda_{j+1}^{j-1}, ..., \Lambda_{n_\tau}^{j-1} \right). \tag{3.17}$$

Notice that $y(0) = F^{(j)}(U^{j-1}, \Lambda^{j-1}) \in B$ and

$$
\begin{aligned}
\| \ y(0) - y^* \ \| &= \max\{\| \ y_Y \ \|_Y, \| \ (y_1, ..., y_{n_\tau}) \ \|_{\mathbb{R}^{n_\tau}} \} = \| \ (y_1, ..., y_{n_\tau}) \ \|_{\mathbb{R}^{n_\tau}} \\
&= \left(\left[\tau_j(U^{j-1}, \Lambda^{j-1}) \right]^2 + \left(\Lambda_{j+1}^{j-1} - \Lambda_{j+1}^* \right)^2 + ... + \left(\Lambda_{n_\tau}^{j-1} - \Lambda_{n_\tau}^* \right)^2 \right)^{1/2} \\
&\geq \left(\left(\Lambda_{j+1}^{j-1} - \Lambda_{j+1}^* \right)^2 + ... + \left(\Lambda_{n_\tau}^{j-1} - \Lambda_{n_\tau}^* \right)^2 \right)^{1/2} = \| \ y(1) - y^* \ \|, \tag{3.18}
\end{aligned}
$$

i.e., $y(1)$ is not farther from the center y^* of the ball B than $y(0)$. Hence $y(1) \in B$, and so $y([0,1])$, which is a rectilinear segment, is contained in B. This implies, first, that $y([0,1])$ is in the domain of H, hence $x(s)$ is well defined, and, second, that $x([0,1]) = H(y[0,1])) \subset W^{(j-1)}$ is an arc, since H is a diffeomorphism and $y([0,1])$ is a rectilinear segment.

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Notice that $x(1) \in W^{(j)} \cap S_j$. Therefore, by assumption, there exists a continuous piecewise smooth curve $x^{(j)}(s)$, $s \in [0,1]$, such that $x^{(j)}(0) = x(1)$, $x^{(j)}(1) = (U^*, \Lambda^*)$, and the conditions (i$_j$) - (iv$_j$) are satisfied. Define

$$
x^{(j-1)}(s) = \begin{cases} x(2s), & 0 \le s < 1/2, \\ x^{(j)}(2s-1), & 1/2 \le s \le 1. \end{cases} \tag{3.19}
$$

By construction, $x^{(j-1)}(s)$ is continuous, piecewise smooth, and $x^{(j-1)}([0,1]) \subset W^{(j-1)}$. Also $x^{(j-1)}([0,1])$ consists of $n_\tau - j + 1$ arcs, since $x^{(j-1)}([0,\frac{1}{2}]) = x([0,1])$ is an arc, whereas $x^{(j-1)}([\frac{1}{2},1]) = x^{(j)}([0,1])$ was assumed to consist of $n_\tau - j$ arcs. More precisely, if $s_j^{(j)}, ..., s_{n_\tau}^{(j)}$ are such as assumed in (iii$_j$), then we define $s_{j-1}^{(j-1)} = 0$, $s_k^{(j-1)} = (s_k^{(j)} + 1)/2$, $k = j, ..., n_\tau$ (clearly, $0 \le s_{j-1}^{(j-1)} \le s_j^{(j-1)} \le ... \le s_{n_\tau}^{(j-1)} = 1$). Then $\mathcal{A}_j^{(j-1)} \equiv x^{(j-1)}([s_{j-1}^{(j-1)}, s_j^{(j-1)}]) = x^{(j-1)}([0,\frac{1}{2}]) = x([0,1])$ and, for $k = j+1, ..., n_\tau$, $\mathcal{A}_k^{(j-1)} \equiv x^{(j-1)}([s_{k-1}^{(j-1)}, s_k^{(j-1)}]) = x^{(j-1)}([\frac{s_{k-1}^{(j)}+1}{2}, \frac{s_k^{(j)}+1}{2}]) = x^{(j)}([s_{k-1}^{(j)}, s_k^{(j)}]) = \mathcal{A}_k^{(j)}$ are arcs. Thus condition (i$_{j-1}$) is satisfied.

Condition (ii$_{j-1}$) is satisfied for $x^{(j-1)}(s)$, since it is satisfied for both $x(s)$ and $x^{(j)}(s)$.

If $x \in \mathcal{A}_j^{(j-1)}$, i.e. $x = x(s)$ for some $s \in [0,1]$, then, for $m = 1, ..., j-1$, $\tau_m(x) = F_m^{(j)}(x) = F_m^{(j)}(x(s)) = F_m^{(j)}(H(y(s))) = y_m(s) = 0$. If $x \in \mathcal{A}_k^{(j-1)}$ for some $k \in \{j+1, ..., n_\tau\}$, then, since $\mathcal{A}_k^{(j-1)} = \mathcal{A}_k^{(j)}$, we have $\tau_1(x) = ... = \tau_{k-1}(x) = 0$ by (iii$_j$). Thus (iii$_j$) holds.

To verify (iv$_{j-1}$) for $x^{(j-1)}(s)$, one has to consider $s \in [0, \frac{1}{2})$ only, since, for $s \in [\frac{1}{2}, 1]$, $x^{(j-1)}(s) = x^{(j)}(2s-1)$, and (iv$_j$) applies. If $s \in [0, \frac{1}{2})$, then $x^{(j-1)}(s) = x(2s)$, so, from the definition of $x(s)$, $\tau_1\left(x^{(j-1)}(s)\right) = ... = \tau_{j-1}\left(x^{(j-1)}(s)\right) = 0$. Thus the implication in (iv$_{j-1}$) has to be verified for $k \ge j$ only. Suppose that $\tau_j\left(x^{(j-1)}(0)\right) \equiv \tau_j(U^{j-1}, \Lambda^{j-1}) \ne 0$ (otherwise the arc $x([0,1])$ degenerates into a single point $x^{(j-1)}(\frac{1}{2})$, which has already been considered. Then, for any $s \in [0, \frac{1}{2})$,

$$
\tau_j(x(2s)) = \tau_j(H(y(2s))) = F_j^{(j)}(H(y(2s))) = y_j(2s) = (1-2s)\tau_j(U^{j-1}, \Lambda^{j-1}) \ne 0. \tag{3.20}
$$

Let us first verify (iv$_{j-1}$) for $k = j$. For any $x \in X$, its last $n_\tau - j$ coordinates coincide with those of $F^{(j)}(x)$ by the definition of $F^{(j)}$, c.f. (3.11a). But $F^{(j)}(x(s)) = y(s)$ whose last $n_\tau - j$ coordinates are $\Lambda_{j+1}^{j-1}, ..., \Lambda_{n_\tau}^{j-1}$, respectively. This proves the implication contained in (iv$_{j-1}$) for $k = j$.

Validity of (iv$_{j-1}$) for $k > j$ follows immediately from the above observation that the last $n_\tau - j$ coordinates of $x(s)$, $0 \le s \le 1$, are $\Lambda_{j+1}^{j-1}, ..., \Lambda_{n_\tau}^{j-1}$, respectively.

Remark 5 *It follows from the construction of the curves $x(s)$ in the proofs of Lemmas 1 and 2_j that, when Λ_j is "freed," the value of $\mid \tau_j(x(s)) \mid$ strictly decreases, as s goes from 0 to 1, provided $\tau_j(x(0)) \ne 0$. This is immediate from $\tau_j(x(s)) = F_j^{(j)}(H(y(s))) = y_j(s) = (1 - s)\tau_j(x(0))$.*

Remark 6 *Curves constructed in the proofs of Lemmas 1 and 2_j have finite length. Indeed, they consist of a finite number of arcs of finite length, see Remark 4.*

4 Examples

4.1 Example 1: Homoclinic orbits in a 3-D singular perturbation problem.

We compute a homoclinic orbit for the 3-D system [11]

$$
\begin{aligned}
x' &= (2 - z)a(x - 2) + (z + 2)[\alpha(x - x_0) + \beta(y - y_0)], &\text{(4.1a)}\\
y' &= (2 - z)[d(b - a)(x - 2)/4 + by] + (z + 2)[-\beta(x - x_0) + \alpha(y - y_0)], &\text{(4.1b)}\\
z' &= (4 - z^2)[z + 2 - m(x + 2)] - \epsilon cz, &\text{(4.1c)}
\end{aligned}
$$

where $a = 1$, $b = 1.5$, $c = 2$, $d = -.2$, $m = 1.1845$, $\alpha = .01$, $\beta = 5$, $x_0 = -.1$, $y_0 = -2$. The parameter ϵ is taken as variable. In this case $n_0 = 2$ and $n_1 = 1$ in Equation (2.1). The discretization is orthogonal collocation with piecewise polynomials, using 25 subintervals and 4 collocation points per interval. A relative Newton tolerance of 10^{-8} is used for u and λ.

Step 0. Initialize the problem parameter: $\epsilon = .01$, and the algorithm parameters: $\epsilon_0 = 10^{-4}$, $T = 10^{-2}$, $c_1 = 1$, $c_2 = 0$.

Step 1. Compute a branch of solutions to the equations (2.4), (2.7), (2.11), (2.12a), and

$$
d_0 = \sum_{j=1}^{n_0} c_j q_{0j}, \tag{4.2}
$$

with scalar variables $T, \epsilon_1 \in \mathbb{R}$, $d_0, d_1 \in \mathbb{R}^3$, $\tau_1, \tau_2 \in \mathbb{R}$, in the direction of increasing T until τ_1 crosses zero. There are ten scalar variables in this continuation. Final values are $T = 2.7568$, $\epsilon_1 = 3.509$, and $\tau_2 = .0223$.

Step 2. Fix $\tau_1 = 0$ and free c_1 and c_2 in (4.3). Compute a solution branch to the system (2.4), (2.7), (2.11), (2.12), and (4.3), in the direction of decreasing c_2 until τ_2 crosses zero. There are now eleven free scalar variables. Final values are $c_1 = 1.0$, $c_2 = -1.51 \times 10^{-4}$, $T = 2.7580$, and $\epsilon_1 = 2.548$.

Step 3. The free parameters $c_1, c_2 \in \mathbb{R}$ are replaced by $d_0 \in \mathbb{R}^3$; see Equation (2.6). Fix $\tau_1 = 0$ and free $\epsilon \in \mathbb{R}$ and hence the matrices $Q_0, Q_1, T_0, T_1 \in \mathbb{R}^3 \times \mathbb{R}^3$. Compute a solution branch to (2.4), (2.5a), (2.6), (2.7), (2.9) - (2.11) in the direction of decreasing ϵ_1 (to increase the accuracy of the orbit) until $\epsilon_1 = \epsilon_0$. There are 44 free scalar variables. Terminal values are $\epsilon = .009333142$, $T = 2.7679$, and $\epsilon_1 = 10^{-4}$.

Note, that it took only 2 steps to get $\tau_1 = \tau_2 = 0$, while the general algorithm requires 3 steps to accomplish this. In particular, since τ_1 crossed zero already in the first step, we were able (without changing the total number of free scalar variables) to keep T free in the second step, while $\tau_1 = 0$ was fixed.

4.2 Example 2: Heteroclinic orbits in a 3-D Josephson Junction problem.

A singularly perturbed sine-Gordon equation, modeling magnetic flux quanta ("fluxons") in long Josephson tunnel junctions with nonzero surface impedance,

$$\beta c \phi'''(\xi) - (1 - c^2)\phi''(\xi) - \alpha c \phi'(\xi) + \sin \phi(\xi) - \gamma = 0, \qquad (4.3)$$

was studied by several authors, see e.g. [5] and references therein. In [14] we computed single and multiple fluxon solutions, which are heteroclinic orbits (or homoclinic orbits on a cylinder). The algorithm in [14] does not allow computation of the transition from two real eigenvalues to a complex conjugate pair. Here we accurately compute this transition point. The three-dimensional first order system is

$$\phi_1' = \phi_2, \qquad (4.4a)$$
$$\phi_2' = \phi_3, \qquad (4.4b)$$
$$\phi_3' = [(1 - c^2)\phi_3 + \alpha c \phi_2 - \sin \phi_1 + \gamma]/\beta c. \qquad (4.4c)$$

We compute a heteroclinic orbit with $u_0 = (\arcsin\gamma, 0, 0)$ and $u_1 = (\arcsin\gamma + \pi, 0, 0)$. Throughout, $\alpha = .18$ and $\beta = .1$ are kept fixed, and γ and c vary. In this case $n_0 = 1$ and $n_1 = 2$ in Equation (2.1). Discretization is as in the preceding example.

Step 0. Initialize the problem parameters, $\gamma = .1$, $c = .6$, and the algorithm parameters, $\epsilon_0 = 10^{-4}$, $\epsilon_1 = .6283$, $T = 10^{-2}$, and $c_1 = 1$.

Step 1. Compute a solution branch to (2.4), (2.7), (2.11), (2.12a), (4.2), with scalar variables $T, \epsilon_1 \in \mathbb{R}$, $d_0, d_1 \in \mathbb{R}^3, \tau \in \mathbb{R}$, in the direction of increasing T until τ crosses zero. There are nine free scalar variables. Terminal values are $T = 9.336$, and $\epsilon_1 = 3.642$.

Step 2. Fix $\tau_1 = 0$. Free $c \in \mathbb{R}$, and hence the matrices $Q_0, Q_1 \in \mathbb{R}^3 \times \mathbb{R}^3$, and the entries $t_{11}^0, t_{12}^0, t_{13}^0, t_{22}^0, t_{23}^0, t_{33}^0$ and $t_{11}^1, t_{12}^1, t_{13}^1, t_{22}^1, t_{23}^1, t_{33}^1$ of the matrices $T_0, T_1 \in \mathbb{R}^3 \times \mathbb{R}^3$, respectively, as well as t_1, t_2, in Equation (4.5) below. Compute a branch of solutions to the system (2.4), (2.5a), (2.6) - (2.10), and

$$t_1 = t_{22}^0 - t_{33}^0, \tag{4.5a}$$
$$t_2 = t_{11}^1 - t_{22}^1, \tag{4.5b}$$

in the direction of decreasing ϵ_1, until $\epsilon_1 = \epsilon_0$. This step involves 44 free scalar variables. Terminal values are $c = .3404$, $T = 21.13$, $\epsilon_1 = 10^{-4}$, $\mu_{01} = 1.073$, $\mu_{11} = -2.600$, and $\mu_{12} = -1.047$. Above, $t_{22}^0 = \operatorname{Re}\mu_{02}$, $t_{33}^0 = \operatorname{Re}\mu_{03}$, $t_{11}^1 = \operatorname{Re}\mu_{11}$, $t_{22}^1 = \operatorname{Re}\mu_{12}$. The parameters t_1, t_2 in (4.5) serve as test functions that cross zero when μ_{02} and μ_{03} (and μ_{11} and μ_{12}) are multiple.

Step 3. Fix ϵ_1 and free $\gamma \in \mathbb{R}$. Compute a solution branch with parameters γ and c in the direction of decreasing γ until t_1 and t_2 cross zero. The equations are as in Step 2. Terminal values are $\gamma = 4790$, $c = .3404$, $T = 12.92$, $\mu_{01} = 1.622$, and $\mu_{11} = \mu_{12} = -2.534$. The double eigenvalue was located with accuracy 10^{-8}.

Step 4. To continue the complex conjugate pair of the eigenvalues, fix $t_1 = t_2 = 0$ ($\operatorname{Re}\mu_{11} = \operatorname{Re}\mu_{12}$) and free t_{32}^0, t_{21}^1 ($\operatorname{Im}\mu_{02}, \operatorname{Im}\mu_{12}$). Compute a solution branch with parameters γ and c to the same system as in Step 3 in the direction of decreasing γ. Final values are $\gamma = 0.8830$, $c = 1.000$, and $T = 30.67$.

Note, that it took only one step to get $\tau = 0$, while the general algorithm requires two steps to accomplish this.

4.3 Example 3: Heteroclinic orbits in a modified 3-D Josephson Junction problem.

Consider system (4.4) with reversed time,

$$\phi_1' = -\phi_2, \tag{4.6a}$$
$$\phi_2' = -\phi_3, \tag{4.6b}$$
$$\phi_3' = -[(1-c^2)\phi_3 + \alpha c\phi_2 - \sin\phi_1 + \gamma]/\beta c. \tag{4.6c}$$

We compute a heteroclinic orbit with $u_0 = (\arcsin\gamma + \pi, 0, 0)$ and $u_1 = (\arcsin\gamma, 0, 0)$. As before, $\alpha = .18$ and $\beta = .1$ are kept fixed, and γ and c vary. The problem parameters are chosen so that $n_0 = 2$ and $n_1 = 1$ in Equation (2.1), where μ_{01} and μ_{02} are a complex conjugate pair of eigenvalues. Discretization is as in the preceding example.

In this problem the starting direction of trajectories near u_0 is unknown, making it difficult to generate a starting orbit in Step 0 with $u(1)$ in a small neighborhood of u_1. Indeed, this example also illustrates the more global applicability of the successive continuation approach.

Step 0. Initialize the problem parameters, $\gamma = .608$, $c = -.95$, and the algorithm parameters, $\epsilon_0 = 10^{-4}$, $\epsilon_1 = .6283$, $T = 10^{-2}$, and $c_1 = 1$, $c_2 = 0$. Initially $\operatorname{Re}\mu_{01} = \operatorname{Re}\mu_{02} = 1.508$, $\operatorname{Im}\mu_{01} = -\operatorname{Im}\mu_{02} = 1.388$.

Step 1. Compute a solution branch to (2.4), (2.7), (2.11), (2.12a), (4.2), with scalar variables $T, \epsilon_1 \in \mathbb{R}$, $d_0, d_1 \in \mathbb{R}^3$, $\tau_1, \tau_2 \in \mathbb{R}$, in the direction of increasing T until τ_2 crosses zero. There are ten free scalar variables. Terminal values are $T = 6.098$, and $\epsilon_1 = 6.1738$, $\tau_1 = -.9500$.

Step 2. Compute a solution branch to (2.4), (2.7), (2.11), (2.12), (4.2), with scalar variables $T, \epsilon_1 \in \mathbb{R}$, $d_0, d_1 \in \mathbb{R}^3$, $c_1, c_2, \tau_1 \in \mathbb{R}$, in the direction of increasing T. There are nine free scalar variables. Terminal values are $T = 9.069$, $\epsilon_1 = 1.737$, and $\tau_1 = -.3718$.

Step 3. Fix ϵ_1. Free $c \in \mathbb{R}$, and hence the matrices $Q_0, Q_1 \in \mathbb{R}^3 \times \mathbb{R}^3$, and the entries $t_{11}^0, t_{12}^0, t_{13}^0, t_{21}^0, t_{22}^0, t_{23}^0, t_{33}^0$ and $t_{11}^1, t_{12}^1, t_{13}^1, t_{22}^1, t_{23}^1, t_{32}^1, t_{33}^1$ of the matrices $T_0, T_1 \in \mathbb{R}^3 \times \mathbb{R}^3$, respectively. Compute a branch of solutions to the system (2.4), (2.5a), (2.6) - (2.10), and

$$t_1 \equiv t_{11}^0 - t_{22}^0 = 0, \tag{4.7a}$$
$$t_2 \equiv t_{22}^1 - t_{33}^1 = 0, \tag{4.7b}$$

in the direction of decreasing $|\tau_1|$ until τ_1 crosses zero. This step involves 44 free scalar variables. Terminal values are $c = -.8995$, $T = 7.436$. Above, $t_{11}^0 = \operatorname{Re}\mu_{01}$, $t_{22}^0 = \operatorname{Re}\mu_{02}$, $t_{22}^1 = \operatorname{Re}\mu_{12}$, $t_{33}^1 = \operatorname{Re}\mu_{13}$.

Step 4. Fix $\tau_1 = 0$ and free $\epsilon_1 \in \mathbb{R}$. Compute a branch of solutions in the direction of decreasing ϵ_1, until $\epsilon_1 = \epsilon_0$. The equations are as in Step 3. Terminal values are $c = -.9027$, $T = 13.16$, $\epsilon_1 = 10^{-4}$.

Note that, as in the general algorithm, it took three steps to get $\tau_1 = \tau_2 = 0$.

4.4 Example 4: Heteroclinic orbits in a 4-D singular perturbation problem.

The existence of traveling wave front solutions to the singularly perturbed reaction-diffusion system

$$v_t = v_{xx} + v(v - a)(1 - v) - w, \quad w_t = \delta w_{xx} + \epsilon(v - \gamma w), \qquad (4.8)$$

for small positive ϵ and δ, was established by Deng [12]. In moving coordinates, $v_1 = v(z)$, $v_2 = v'(z)$, $w_1 = w(z)$, $w_2 = w'(z)$ with $z = t + cx$, the reduced ODE is

$$
\begin{align}
v_1' &= v_2, \tag{4.9a}\\
v_2' &= cv_2 - v_1(1 - v_1)(v_1 - a) + w_1, \tag{4.9b}\\
w_1' &= w_2, \tag{4.9c}\\
w_2' &= [cw_2 - \epsilon(v_1 - \gamma w_1)]/\delta. \tag{4.9d}
\end{align}
$$

We compute a heteroclinic orbit with $u_0 = (0, 0, 0, 0)$ and $u_1 = (\frac{1}{2} + \frac{1}{2}a + \frac{1}{2}\sqrt{(\gamma - 2a\gamma + \gamma a^2 - 4)/\gamma}, 0, v_1/\gamma, 0)$, with $\delta = \epsilon = .001$ and $a = .3$ fixed and and γ and c variable. Initially $\gamma = 13.8$ and $c = .257$. In this case $u_1 = (.8736878, 0, .0633107, 0)$, and $n_0 = n_1 = 2$, where the relevant eigenvalues are $\mu_{0,1} = .6957$, $\mu_{0,2} = 257.0537$, $\mu_{1,1} = -.4415$, and $\mu_{1,2} = -0.0668$. Throughout we use a discretization with 50 subintervals, 4 collocation points per interval and relative Newton tolerances 10^{-8} for u and λ.

In this problem there is strong divergence of trajectories near u_0, making it difficult to generate a starting orbit in Step 0 with $u(1)$ in a small neighborhood of u_1. Indeed, this example also illustrates the continued applicability of the algorithm to such cases.

Step 0. Initialize the problem parameters, $\gamma = 13.8$, $c = .2570$, and the algorithm parameters, $\epsilon_0 = .6$, $\epsilon_1 = .5161$, $T = 10^{-5}$, $c_1 = 1$, $c_2 = 0$.

Step 1. Compute a solution branch to (2.4), (2.7), (2.11), (2.12a), (4.3), with scalar variables $T, \epsilon_1, \tau_1, \tau_2 \in \mathbb{R}$, $d_0, d_1 \in \mathbb{R}^4$, in the direction

of increasing T until τ_1 crosses zero. Terminal values are $T = .0472$ and $\epsilon_1 = .5056$.

Step 2. Fix $\tau_1 = 0$, free c_1 and c_2, and compute a solution branch to (2.4), (2.7), (2.11), (2.12), (4.3), in the direction of increasing T, with scalar variables $T, \epsilon_1, \tau_2, c_1, c_2 \in \mathbb{R}$, $d_1 \in \mathbb{R}^4$. Final values are $T = 1.363$, $\epsilon_1 = .4024$, $c_1 = 1.00000$, $c_2 = 1.9 \times 10^{-8}$, and $\tau_2 = .521$.

Step 3. The scalar variables and equations are as in Step 2, except that T is fixed and ϵ_0 is free. Compute a branch of solutions in the direction of decreasing ϵ_0 and ϵ_1 to locate zero of τ_2. Terminal values are $\epsilon_0 = .3199$, $\epsilon_1 = .3991$, $c_1 = 1.00000$, and $c_2 = 1.3 \times 10^{-8}$. There is a very sensitive dependence on the "shooting angle", represented by c_2.

Step 4. The free parameters $c_1, c_2 \in \mathbb{R}$ are replaced by $d_0 \in \mathbb{R}^4$. Fix $\tau_2 = 0$ and free T. Also free the problem parameter $c \in \mathbb{R}$, and hence the matrices $Q_0, Q_1, T_0, T_1 \in \mathbb{R}^4 \times \mathbb{R}^4$. Compute a solution branch to the system (2.4)-(2.10) in the direction of increasing T. Terminal values are $c = .3437209$, $T = 12.66$, and $\epsilon_0 = 10^{-4}$.

Step 5. The scalar variables and equations are as in Step 4, except that ϵ_0 is fixed and ϵ_1 is free. Compute a solution branch in the direction of increasing T. Final values are $c = .2572501$, $T = 71.31$, $\epsilon_1 = 5 \times 10^{-3}$.

5   Discussion

The initial detection of a connecting orbit in a dynamical system is generally a difficult task; often with extremely sensitive dependence on initial conditions and on parameter values. This is even more so in the case of singularly perturbed equations. Thus there is use for a systematic procedure that has a good chance of success, even in difficult problems. In this paper we have presented a successive continuation method for locating connecting orbits. We have shown that the procedure works, provided the connecting orbit is isolated and the initial orbit sufficiently close. Thus our analysis only guarantees local convergence of the method, even though it has been designed for extended convergence properties, as is well illustrated by our numerical examples, which include some "hard" problems. A complete presentation of global convergence properties is beyond the scope of this paper, and perhaps best presented in a more general context. The key ideas in a global analysis of the successive continuation algorithm are the following. It is assumed that

the problem can be reduced to that of finding a small number of parameters for which an equal number of equations is to be satisfied. Given a subset of the equations that are satisfied, a one-dimensional continuum of such solutions is followed, and points where any of the remaining equations are satisfied are accurately located. Proceeding, inductively, one then continues an enlarged set of satisfied equations. At any stage of the algorithm, the continuation procedure works locally, provided the solution points are "regular" [16]. Generically this is the case, while for nongeneric problems (which are often encountered!) one can regularize the problem by adding (if necessary) unfolding parameters and (again, if necessary) regularizing equations. In fact, the method of pseudo-arclength continuation itself is the simplest nontrivial example of this procedure.

The power of the successive continuation procedure is then its ability to reach a solution from a far away starting point, and, in fact, to locate multiple solutions and often all solutions, provided the regularity assumptions are satisfied and provided *the solution(s) are reachable.* It is the latter condition that need not always be satisfied. In fact, it is easy to construct simple (algebraic) examples where a solution is not reachable from a given starting point. One could argue that this problem can also be solved by adding unfolding parameters, but in practice it is not often clear how to do this, for example, in the case of computing connecting orbits. Nevertheless, as our numerical experience has shown, including the examples presented in this paper, the successive continuation method provides, at least, a useful tool that often gives results where other methods fail.

Note that, in our computation of connecting orbits, the above reduction to a "small-dimensional problem" does not require the problem to be posed as a "shooting problem", which would make the algorithm useless, for example, for the singular perturbed equation in Section 4.1. Throughout, the small dimensional problem remains embedded in the full set of equations, which are solved by continuation in the full space. Even the initial "integration" (see Algorithm, Step 1) is done by continuation of complete orbits, in order to be able to monitor, and react to (e.g. adaptive mesh refinement), sensitive dependence, for example, on the left boundary conditions.

Although, as pointed out above, a discussion of global convergence properties is perhaps best presented in terms of the global topology of the underlying manifolds, one can also obtain global results by making certain global assumptions on the vector field, although this is practically less useful in the present context. In fact, applying the theory in [25], one can show the

following. Let $F_h^{(n_\tau)} : X_h \to Y_h \times \mathbb{R}^{n_\tau}$ be the discretization [16, pp. 748-749] of $F^{(n_\tau)} : X \to Y \times \mathbb{R}^{n_\tau}$ defined by (3.11b). Let $\Omega \subset X_h$ be a bounded open set with a smooth connected boundary $\partial\Omega$. Suppose that the operator $F_h^{(n_\tau)}$ satisfies Smale boundary conditions [25]

    a) $D_U F_h^{(n_\tau)}(U_h, \Lambda_h)$ is nonsingular on $\partial\Omega$; and either

    b) $(D_U F_h^{(n_\tau)}(U_h, \Lambda_h))^{-1} F_h^{(n_\tau)}(U_h, \Lambda_h)$ points into Ω, $\forall U_h \in \partial\Omega$; or

    c) $(D_U F_h^{(n_\tau)}(U_h, \Lambda_h))^{-1} F_h^{(n_\tau)}(U_h, \Lambda_h)$ points out of Ω, $\forall U_h \in \partial\Omega$.

Then by a slight generalization of [25, Th. 2.4] one can show that $\forall U_h^0 \in \partial\Omega$ there exists a piecewise smooth path with starting point (U_h^0, Λ_h^0) and terminal point (U_h^*, Λ_h^*) with $F_h^{(n_\tau)}(U_h^*, \Lambda_h^*) = 0$.

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